ii) determining, using the processor, for each atom in the molecule, a predicted Gibbs free energy of binding of the atom to an ideal ligand for the atom;

iii) generating, using the processor, a three-dimensional prediction model of binding targets in the molecule by generating, using the three-dimensional coordinates of each of the atoms in the molecule, a model of the atoms in the molecule and mapping onto each atom depicted in the model the corresponding determined predicted Gibbs free energy of binding; said generating step yielding data including the identity and three-dimensional coordinates of each of the atoms in the binding target which will be input into the programmed computer,

(b) inputting into the programmed computer, through the input device, data including the identity and three-dimensional coordinates of each of the atoms in [a selected] the compound;

(c) generating, using the processor, a model of the [selected] compound bound to the [selected] binding target [site];

(d) determining, using the processor, the three-dimensional coordinates of an energy minimized structure of the [selected] compound when the [selected] compound is bound to the [selected] binding target [site]; and

(e) determining, using the processor, a predicted binding affinity of the energy minimized [selected] compound for the [selected] binding target [site].

Claim 13. (Amended) A computer program, residing on a computer-readable medium, for predicting the binding affinity of a [selected ligand] compound for [binding to] a [selected] binding target [site] of a [selected] molecule, the computer program including instructions for causing a computer to:

(a) receive data including the identity and three-dimensional coordinates of each of the atoms in [a selected] the binding [site] target [of a selected molecule]; wherein the binding target has been selected from a plurality of predicted binding targets generated by

i) inputting into a programmed computer, through an input device, data including the identity and three-dimensional coordinates of each of the atoms in the molecule;

ii) determining, using a processor, for each atom in the molecule, a predicted Gibbs free energy of binding of the atom to an ideal ligand for the atom;

iii) generating, using the processor, a three-dimensional prediction model of binding targets in the molecule by generating, using the three-dimensional coordinates of each of the atoms in the molecule, a model of the atoms in the molecule and mapping onto each atom depicted in the model the corresponding determined predicted Gibbs free energy of binding; said generating step yielding data including the identity and three-dimensional coordinates of each of the atoms in the binding target which will be input into the programmed computer,

(b) receive data including the identity and three-dimensional coordinates of each of the atoms in [a] the [selected] compound;

(c) generate a model of the [selected] compound bound to the [selected] binding target [site];

(d) determine the three-dimensional coordinates of an energy minimized structure of the [selected] compound when the [selected] compound is bound to the [selected] binding target [site]; and

(e) determine a predicted binding affinity of the energy minimized [selected] compound for the [selected] binding target [site].

REMARKS

Claims 2-4, 6-10, 13, 15 and 17 are pending in the application. Claims 3, 4, 15 and 17 have been withdrawn from consideration. Claims 2, 6-10 and 13 are currently under rejection. By this amendment, the specification has been amended in accordance with the Examiner's requirements, and claims 2 and 13 have been amended.